Ecotox Report for Case # LM-17-0030

General

CBI:
Report Status: Complete
Status Date: 08/30/2017
CRSS Date: 08/31/2017
SAT Date: 09/01/2017
SAT Chair: [redacted]
Consolidated PMN: N
Consolidated Set:
Ecotox Related Cases: [redacted]
Health Related Cases: [redacted]
Submitter: Soulbrain MI
CAS Number: 1072-53-3
Chemical Name: 1,3,2-Dioxathiolane, 2,2-dioxide
Use: [redacted]
Trade Name: ESA, DTD
PV-max(kg/yr): [redacted]
Ecotox Assessor: [redacted]

Fate Summary Statement

Fate Summary Statement: M-17-0030

FATE:
Solid with MP = 96-99 °C (M)
log Kow = -0.90 (E)
S
= 382 mg/L at 25 °C (E)

VP = 0.04 torr at 25 °C (E)
BP = 209 °C
(E)
H = 1.15E-6 (E)
log Koc = 0.97 (E)
log Fish BCF = 0.5 (3)
(E)
log Fish BAF = -0.047 (0.9) (E)
POTW removal (%) = 0-25

Time for complete ultimate aerobic biodeg = mo
Sorption to
soils/sediments = low
Volatilization half-life from a standard river =
570 hrs
Volatilization half-life from a standard lake = 260 da

Atmospheric Oxidation Half-life = 120 hr via OH radical
PBT
Potential: P3B1
*CEB FATE: Migration to ground water = rapid

Bioconcentration factor to be put into E-FAST: 3.2

PMN
Material:
Overall wastewater treatment removal is 0-25% due to low biodegradability, low sorption and low stripping.
Sorption to sludge
is low based on the estimated physical-chemical properties from EPISuite and analogous chemicals.
Air Stripping (Volatilization to air) is
negligible based on the estimated Henry's Law Constant.
Removal by
biodegradation in wastewater treatment is negligible based on BIOWIN model
estimates and analogous chemicals.
The aerobic aquatic biodegradation
half-life is months based on BIOWIN model estimates and analogous chemicals.
The anaerobic aquatic biodegradation half-life is greater
than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater or equal to the aerobic biodegradation half-life.

Sorption to soil and sediment is low based on the estimated PCKOC

model estimates and analogous chemicals.
Migration to groundwater is
rapid based on the estimated PCKOC model estimates and analogous chemicals.
PMN Material:
High Persistence (P3) is based on the
anaerobic biodegradation half-life and analogous chemicals.
Low
Bioaccumulation potential (B1) is based on BCFBAF model estimates.

Bioconcentration/Bioaccumulation factor to be put into E-Fast: BCF: 3.2
NOTE: The chemical may be inherently
biodegradable.

Physical Chemical Information

Molecular Weight:	124.12		
Wt% < 500:		**Wt% < 1000:**	
Physical State - Neat:	Solid		
Melting Point:	96.00 - 99.00	**Melting Point (est):**	
MP (EPI):	99.00		
Vapor Pressure:		**Vapor Pressure (est):**	0.04
VP (EPI):	4.00e-002		
Water Solubility:		**Water Solubility (est):**	382
Water Solubility (EPI):			
Henry's Law::			
Log Koc:		**Log Koc (EPI):**	
Log Kow:		**Log Kow (EPI):**	-0.90
Log Kow Comment:			

SAT Concern Level

Ecotox Rating (1):	2

Ecotox Rating Comment (1):	PMN substance
Ecotox Rating (2):	
Ecotox Rating Comment (2):	
Ecotox Route of Exposure:	No releases to water

Ecotox Comments

Exposure Based Review (Eco):	N
Ecotox Comments:	
Exposure Based Testing:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
3	1	2	

Eco-Toxicity Comment:

Fate Ratings

Removal in WWT/POTW (Overall): 0-25

Condition	Rating Values	Rating Description 1	2	3	4	Comment
Fish BCF:						
Log Fish BCF:						
WWT/POTW Sorption:	1	Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:	4	Extensive	Moderate	Low	Negligible	
Biodegradation Removal:	4	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:		Unknown	Complete	Partial	—	

Removal in WWT/POTW (Overall):	0-25					
Condition	**Rating Values**	**Rating Description**				**Comment**
		1	**2**	**3**	**4**	
Aerobic Biodeg Ult:	3	<= Days	Weeks	Months	> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	4	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes	Hours	Days	>= Months	
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	4	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	4	Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	

Bio Comments: PMN
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negligible based on the estimated Henry's Law Constant.
Removal by
biodegradation in wastewater treatment is negligible based on BIOWIN model
estimates and analogous chemicals.
The aerobic aquatic biodegradation

Removal in WWT/POTW (Overall):	0-25					
Condition	**Rating Values**	**Rating Description** 1	2	3	4	**Comment**
		half-life is months based on BIOWIN model estimates and analogous chemicals. The anaerobic aquatic biodegradation half-life is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater or equal to the aerobic biodegradation half-life. Sorption to soil and sediment is low based on the estimated PCKOC model estimates and analogous chemicals. Migration to groundwater is rapid based on the estimated PCKOC model estimates and analogous chemicals. PMN Material: High Persistence (P3) is based on the anaerobic biodegradation half-life and analogous chemicals. Low Bioaccumulation potential (B1) is based on BCFBAF model estimates. Bioconcentration/Bioaccumulation factor to be put into E-Fast: BCF: 3.2 NOTE: The chemical may be inherently biodegradable.				
Fate Comments:		PMN Material: Overall wastewater treatment removal is 0-25% due to low biodegradability, low sorption and low stripping. Sorption to sludge is low based on the estimated physical-chemical properties from EPISuite and analogous chemicals. Air Stripping (Volatilization to air) is negligible based on the estimated Henry's Law Constant. Removal by biodegradation in wastewater treatment is negligible based on BIOWIN model estimates and analogous chemicals. The aerobic aquatic biodegradation half-life is months based on BIOWIN model estimates and analogous chemicals. The anaerobic aquatic biodegradation half-life is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater or equal to the aerobic biodegradation half-life.				

Removal in WWT/POTW (Overall):	0-25					
Condition	**Rating Values**	**Rating Description** 1	2	3	4	**Comment**
	Sorption to soil and sediment is low based on the estimated PCKOC model estimates and analogous chemicals. Migration to groundwater is rapid based on the estimated PCKOC model estimates and analogous chemicals. PMN Material: High Persistence (P3) is based on the anaerobic biodegradation half-life and analogous chemicals. Low Bioaccumulation potential (B1) is based on BCFBAF model estimates. Bioconcentration/Bioaccumulation factor to be put into E-Fast: BCF: 3.2 NOTE: The chemical may be inherently biodegradable.					

Ecotoxicity Values

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Fish	96-h	LC50	> 100	[redacted]	[redacted]
Daphnid	48-h	LC50	> 100		" "
Green Algae	96-h	EC50	> 100	[redacted]	" "
Fish	-	Chronic Value	> 10		" "
Daphnid	-	Chronic Value	> 10		" "
Green Algae	-	Chronic Value	> 10	[redacted]	" "

Ecotox Value Comments: Predictions are based on QSARs for esters (ECOSAR V2.2); [redacted] Log Kow = -0.90 (P); solid with a MP = 99C (M); S = 382,000 mg/L (P); effective concentrations based on 100% active ingredients and

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
	mean measured concentrations; hardness <150 mg/L as CaCO3; and TOC <2.0 mg/L.				

Ecotox Factors

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Aquatic (ppb):		5/10	5000	Based on algae ChV
Chronic Aquatic (ppb):			500	Based on algae ChV

Factors	Values	Comments
SARs:	Esters	
SAR Class:	Esters	
TSCA NCC Category?	Esters	

Recommended Testing:

Ecotox Factors Comments: Environmental

Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risks because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using the Ecological Structure Activity Relationships (ECOSAR) Predictive Model (https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model).
Based on these estimated hazard values, EPA concludes that this chemical substance has moderate environmental hazard.

· Substance falls
within the TSCA New Chemicals Category of Esters.
· SAR chemical
class of esters.
· Moderate hazard based on acute and chronic COCs of
5,000 and 500 ppb, respectively.

Environmental Risk:
· Risks
were not identified.

Testing Recommendations:
· No testing recommended.

Comments/Telephone Log

Artifact	Update/Upload Time